





# Tightly Coupled Mechanistic Study of Materials in the Extreme Space Environment

2012 Space Propulsion and Power Program Review

10-14 September 2012, Arlington VA

Deborah A. Levin, Adri van Duin, Krishna Rajan, Raymond Sedwick and Mark Lewis

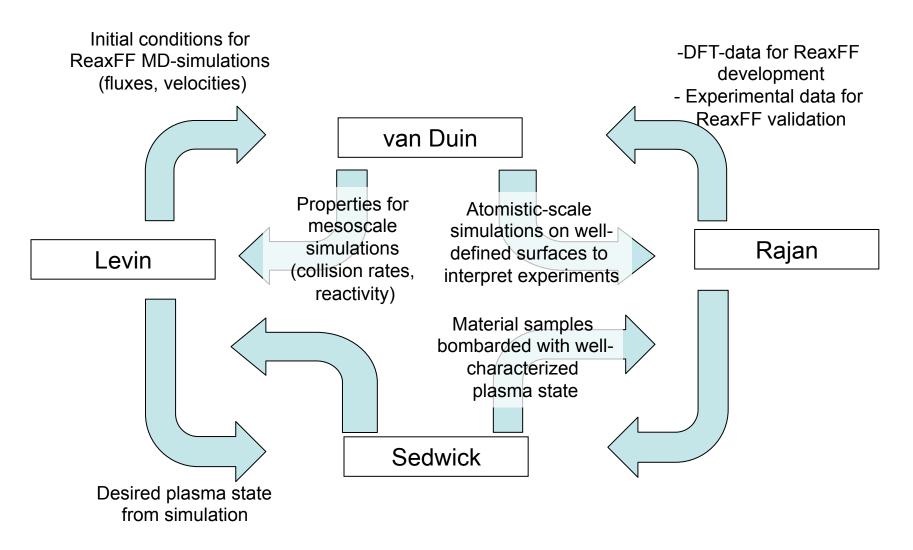
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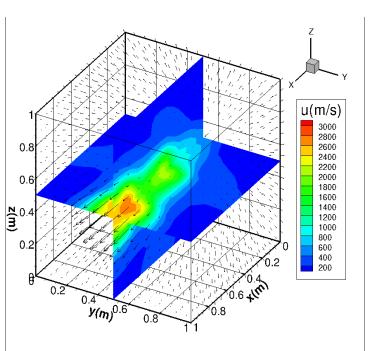
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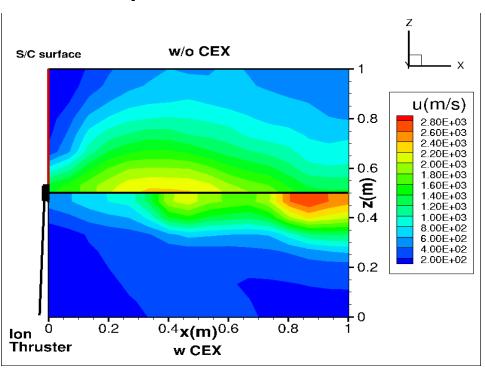
#### Connections in this project





#### D. Levin – PRELIMINARY CEX 3-D Multi-step Results

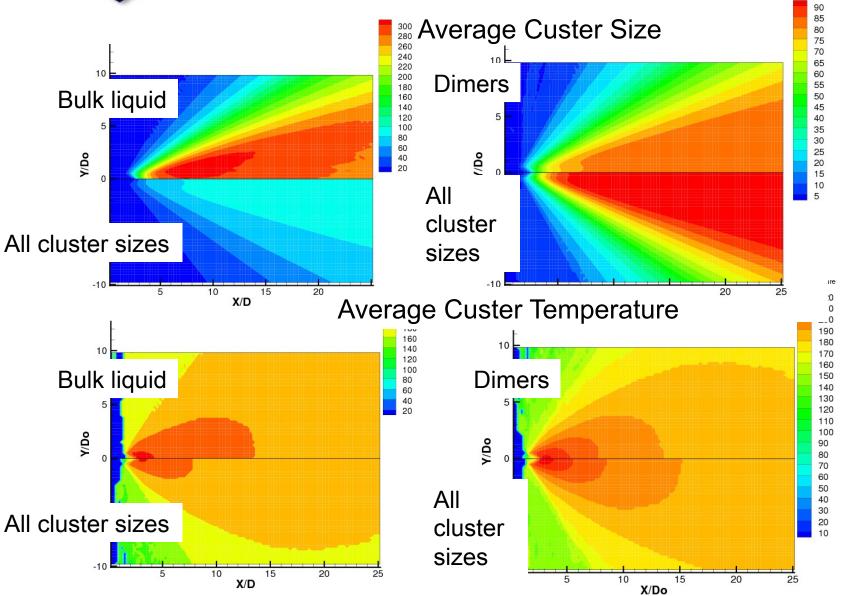




- It is apparent that cross-species interaction results in a much complex plume structure than for a pure neutral flow. The energy exchange causes neutral species to achieve much higher speeds.
- The energy deposited by the ions into neutrals results in a lower expansion angle since directional velocity for neutrals are greatly increased when CEX reactions are present.

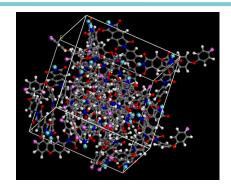


# Sensitivity of DSMC Condensating Flows to Cluster Latent Heat Models

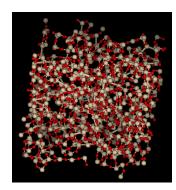


# Simulations - A.C.T. Van Duin and A.Rahnamoun - ReaxFF force field

✓ Kapton structure



✓ Silica structure

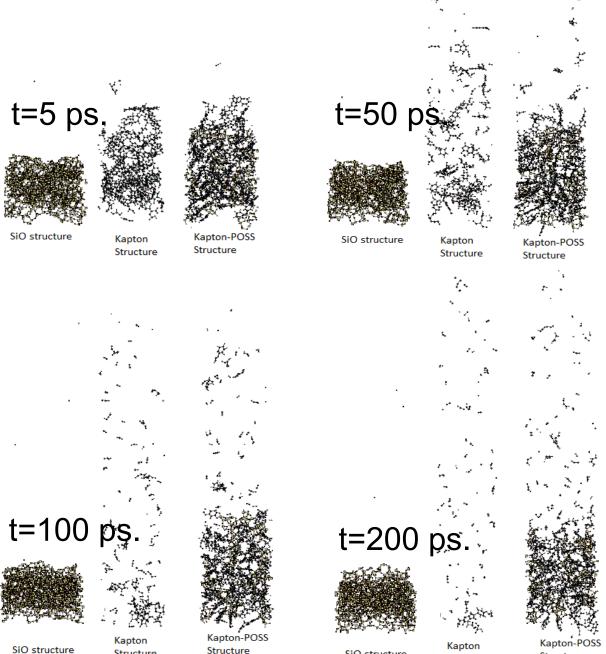


✓POSS(Polyhedral Oligomeric Silsesquioxane) - Kapton structure mixed with silica side-chains

#### **ReaxFF Generated Sequence of Hypervelocity Surface Impact Events**

Structure

- √8 ev bombardment energy
- √ Time step in the simulation is 0.1 fs
- √ Frequency of high energy oxygen addition is every 2000 iterations (2ps)
- ✓ Disintegration rate: Kapton > POSS >> Silica
- POSS bombardment leads to silica clustering
- -Main Kapton decomposition products: carbon monoxide and formaldehyde
- Simulations can be used to define optimal silica addition to Kapton
- Ongoing simulations: water cluster t=100 ps bombardment of silica surfaces

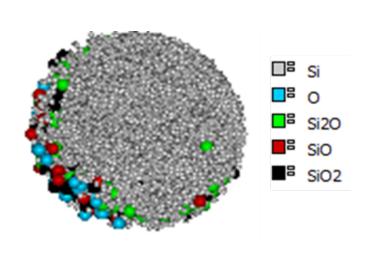


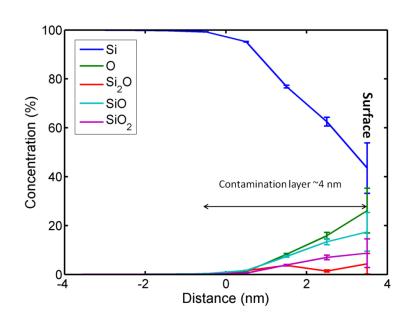
SiO structure

Structure

Structure

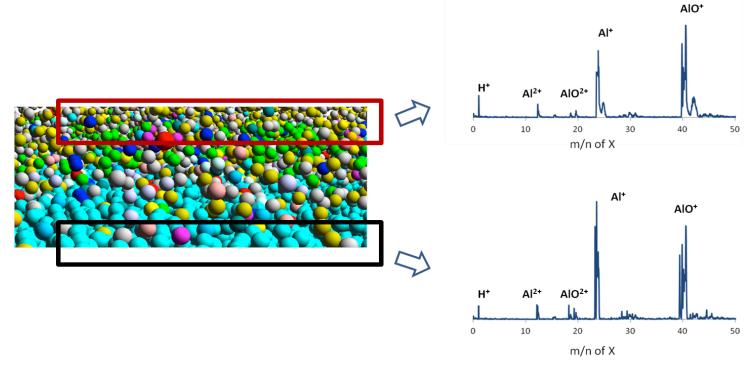
#### **Atom probe tomography: Si / Silica/ Oxygen Reactions**





- A cross section image of the specimen showing the degradation of silicon due to silicon-oxygen reaction at the surface was taken.
- The concentration profile across the Si-Oxide interface measuring surface chemistry and the diffusion of gas into the material was made.
- The ratio of O:Si-O compounds decreases with diffusion distance, implying that the metal-gas reactions and subsequent bond strengths are strongest at the metal-gas interface, while the resulting surface atoms are more weakly bonded to material.

#### Atom probe tomography: Al / Alumina/ Oxygen Reactions



- ➤ Measurement of pair wise interactions between Al and other atoms / compounds at the atomic scale.
- ➤ The top spectra describes the compounds and corresponding valencies that degrade concurrent with Al<sup>+</sup> atom in the alumina region at the interface; the bottom spectra is the same except in the Al region near the interface.
- ➤ This map allows us to understand the complexity of the chemical states and identify the differences in bonding and inter-atomic interactions. The differences in the spectra represent changes in material degradation between phases at the metal surface, and describe the strength of inter-atomic interactions and mechanism for gas-solid reaction.

### Material bombardment with well-characterized plasma state – Plasma Sources

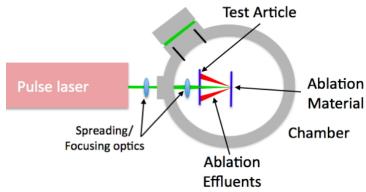


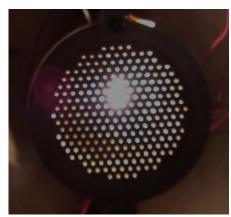


- Ion Engine Simulator Completed, under test
  - Characteristic ion energy/density and neutral density
  - Also can be used for validation of CEX modeling
- Gen-II IonEtch sputter ion Gun Available for testing
  - Microwave source supports reactive species
  - Energies up to 5 keV
- Dusty Plasma Source Currently under design
  - AFOSR Funded DURIP
  - Will use laser ablation to generate both atoms and particulates/droplets from solids/liquids



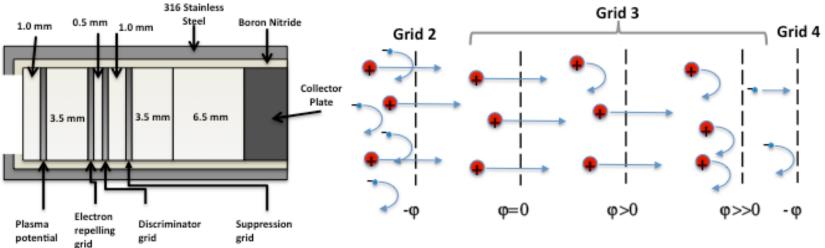




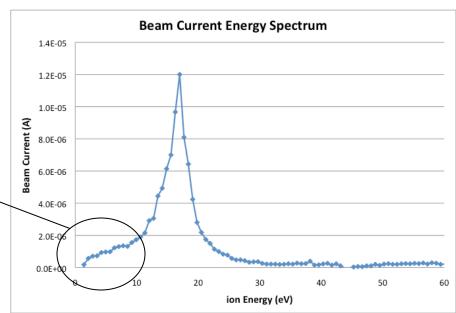


## Ion energy spectrum analysis – Retarding Potential Analyzer





- RPA used to determine beam energy spectrum
- Spatially resolving ion energy distribution can characterize CEX reactions
  - Lower energy ions appear farther from the exit plane and centerline
- For dusty plasma source, TOF will also be employed to determine charge-to-mass distribution as well



### First Batch of Silicon tip coupons being shipped to UMD from Iowa State

- Each coupon contains 36 (6x6) individual presharpened micro-tips
- Each tip is sharpened to a point less than 50 nm in diameter and is 100 microns (+/-20) in height
- Coupon are 3 mm x 7 mm and come on a gel pack





Prior to testing with coupons, small blanks will be used and analyzed with an SEM

 This will help to establish minimum and maximum exposure times for coupon testing

Coupons will be temporarily mounted to a backing plate during testing and then returned to the gel pack

